

Phase diagram of spin-1/2 bosons in one-dimensional optical lattice

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Systems of two coupled bosonic species are studied using Mean Field Theory and Quantum Monte Carlo. The phase diagram is characterized both based on the mobility of the particles (Mott insulating or superfluid) and whether or not the system is magnetic (different populations for the two species). The phase diagram is shown to be population balanced for negative spin-dependent interactions, regardless of whether it is insulating or superfluid. For positive spin-dependent interactions, the superfluid phase is always polarized, the two populations are imbalanced. On the other hand, the Mott insulating phase with even commensurate filling has balanced populations while the odd commensurate filling Mott phase has balanced populations at very strong interaction and polarizes as the interaction gets weaker while still in the Mott phase.

PACS numbers: 05.30.Jp, 03.75.Hh, 67.40.Kh, 75.10.Jm 03.75.Mn

I. INTRODUCTION

When ultra-cold bosonic atoms with internal degrees of freedom, *e.g.* ^{87}Rb or ^{23}Na in $F = 1$ hyperfine state, are confined in magneto-optical traps, the magnetic field aligns the spins and the system behaves effectively as one of spin-0 particles. Progress in purely optical trapping techniques now allows the confinement of these atoms with their full spin degrees of freedom present [1, 2] which permits the study of the interplay between magnetism and superfluidity. In such systems, in addition to the usual spin-independent contact interaction, there are spin-dependent terms [3] and also longer range interactions [4]. Mean field calculations [3] in the absence of the long range interactions, show that the interactions can be ferromagnetic (*e.g.* ^{87}Rb) or antiferromagnetic (*e.g.* ^{23}Na), depending on the relative magnitudes of the scattering lengths in the singlet and quintuplet channels. When loaded in an optical lattice, the system is governed by an extended Hubbard Hamiltonian with spin-dependent and spin-independent terms. The phase diagram in the mean field and variational approximations has been calculated at zero [5–8] and at finite temperature [8].

The overall picture emerging from these calculations is that in the ferromagnetic case, *i.e.* negative spin-dependent interaction, the system is in a Mott insulating (MI) phase when the filling is commensurate with the lattice size and the repulsive contact interaction is strong enough. When this interaction is weaker, or when the particle filling is incommensurate, the system is in a ferromagnetic superfluid (SF) phase. The SF-MI transitions in the ground state are all expected to be continuous. Furthermore, all Mott lobes shrink, and eventually disappear, as the ratio of the spin-dependent interaction to the spin-independent one increases. These predictions have been confirmed for the one-dimensional case with Quantum Monte Carlo (QMC) simulations [9].

The phase diagram for the antiferromagnetic case also

has MI lobes at commensurate fillings and strong coupling and a SF phase at weak coupling or incommensurate fillings. However, the nature of the SF phase and the MI-SF transitions are different. In this case, the SF phase is “polar”: Superfluidity is carried either by the $S_z = 0$ component or by the $S_z = \pm 1$ components. Furthermore, the Mott lobes of odd order are expected to be nematic in two and three dimensions and dimerized in one dimension [5]. The MI-SF transition into these odd Mott lobes is generally expected to be continuous. In the even Mott lobes, the bosons are predicted to be in a singlet state which is expected to increase the stability of the MI. This transition from non-singlet SF to singlet MI is argued to render the transition into the even Mott lobes of first order. Density Matrix Renormalization Group (DMRG) [10, 11] and QMC [12] calculations for one-dimensional systems have confirmed the dimerized nature of odd lobes, and determined the phase diagram. Further QMC work [9] presented evidence of singlet formation in the even lobes but did not find clear evidence of first order phase transitions.

A related model is obtained by coupling degenerate atomic ground states and degenerate excited states (see next section) to yield a system of two bosonic species sometimes referred to as spin-1/2 bosons [13, 14]. As for the full spin-1 case, the spin-dependent interaction can be ferromagnetic or antiferromagnetic. Mean field analysis of this model [13] yielded phase diagrams which are rather similar to the spin-1 case. In this paper we shall present an extension of previous mean field treatments [13] which yields better qualitative agreement with exact QMC simulations, which we also present for the one-dimensional system. The paper is organized as follows: In Sec. II the Hamiltonian of two bosonic species is presented. The Mean Field phase diagram is discussed in Sec. III. Finally, in Sec. IV Quantum Monte Carlo calculations on one dimensional lattices verify the qualitative conclusions of the Mean Field theory (MFT), but provide quantitatively accurate values for the phase boundaries.

II. TWO BOSONIC SPECIES HAMILTONIAN

We follow Ref. [13] and consider a system of neutral polarizable bosonic atoms with three degenerate internal ground states ($F_g = 1$) and excited states ($F_e = 1$) characterized by the magnetic quantum number $S_z = 0, \pm 1$. The atoms are loaded in a d -dimensional optical lattice produced by counterpropagating laser beams. As explained in Ref. [13], in addition to generating the optical lattice, the lasers can be used to couple the internal ground and excited states by V and Λ transitions leading to two sets of orthogonal Bloch eigenmodes denoted respectively by 0 and Λ [13]. The resulting Bose Hubbard Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(a_{\sigma i}^\dagger a_{\sigma j} + a_{\sigma j}^\dagger a_{\sigma i} \right) + \frac{U_0}{2} \sum_{\sigma, i} \hat{n}_{\sigma i} (\hat{n}_{\sigma i} - 1) + \frac{U_2}{2} \cos(\delta\phi) \sum_i \left(a_{0i}^\dagger a_{0i}^\dagger a_{\Lambda i} a_{\Lambda i} + a_{\Lambda i}^\dagger a_{\Lambda i}^\dagger a_{0i} a_{0i} \right) + (U_0 + U_2) \sum_i \hat{n}_{0i} \hat{n}_{\Lambda i} - \mu \sum_{\sigma, i} \hat{n}_{\sigma i}, \quad (1)$$

where $a_{\sigma i}^\dagger$ ($a_{\sigma i}$) creates (annihilates) a particle of “spin” $\sigma = 0, \Lambda$ on site i , $U_0 > 0$ is the spin-independent contact repulsion term and U_2 is the spin-dependent interaction term. The number operator, $\hat{n}_{\sigma i}$, counts the number of particles of type σ on site i and μ is the chemical potential. We take the hopping parameters $t = 1$ to set the energy scale. The phase difference, $\delta\phi = 2(\phi_0 - \phi_\Lambda)$, gives the relative global phase between the two species. Equation (1) is the same as Eq. (9) of Ref. [13] after one uses Eqs. (13) and (15) of that reference. The relative phase, $(\phi_0 - \phi_\Lambda)$, was then determined by the requirement that the total energy be minimized. It was argued in Ref. [13] that since U_2 can be positive or negative, the way to minimize the energy is to have the coupling in the third term of Eq. (1) be of the form $-|U_2|/2$. This gives $\phi_0 = \phi_\Lambda$ for $U_2 < 0$ and $\phi_0 = \phi_\Lambda \pm \pi/2$ for $U_2 > 0$. The Hamiltonian then becomes

$$H_1 = -t \sum_{\langle i,j \rangle, \sigma} \left(a_{\sigma i}^\dagger a_{\sigma j} + a_{\sigma j}^\dagger a_{\sigma i} \right) + \frac{U_0}{2} \sum_{\sigma, i} \hat{n}_{\sigma i} (\hat{n}_{\sigma i} - 1) - \frac{|U_2|}{2} \sum_i \left(a_{0i}^\dagger a_{0i}^\dagger a_{\Lambda i} a_{\Lambda i} + a_{\Lambda i}^\dagger a_{\Lambda i}^\dagger a_{0i} a_{0i} \right) + (U_0 + U_2) \sum_i \hat{n}_{0i} \hat{n}_{\Lambda i} - \mu \sum_{\sigma, i} \hat{n}_{\sigma i}. \quad (2)$$

However, this is not the only possible solution: The sign of the third term has no effect on the energy and the Hamiltonian obtained by putting $\phi_0 = \phi_\Lambda$ both for U_2

positive or negative,

$$H_2 = -t \sum_{\langle i,j \rangle, \sigma} \left(a_{\sigma i}^\dagger a_{\sigma j} + a_{\sigma j}^\dagger a_{\sigma i} \right) + \frac{U_0}{2} \sum_{\sigma, i} \hat{n}_{\sigma i} (\hat{n}_{\sigma i} - 1) + \frac{U_2}{2} \sum_i \left(a_{0i}^\dagger a_{0i}^\dagger a_{\Lambda i} a_{\Lambda i} + a_{\Lambda i}^\dagger a_{\Lambda i}^\dagger a_{0i} a_{0i} \right) + (U_0 + U_2) \sum_i \hat{n}_{0i} \hat{n}_{\Lambda i} - \mu \sum_{\sigma, i} \hat{n}_{\sigma i}, \quad (3)$$

yields exactly the same free energy as Eq. (2). For the $U_2 < 0$ case, this is obvious since Eq. (2) is identical to Eq. (3). For $U_2 > 0$, this can be seen by writing the partition function, $Z = \text{Tr} e^{-\beta H}$, and noting that if we expand the exponential in powers of the term in question, only even powers will contribute. In fact, for $U_2 > 0$, one can transform Eq. (2) into Eq. (3) by a simple phase transformation, $a_{0i} \rightarrow a_{0i} e^{i\pi/2}$. Therefore, both Eqs. (2) and (3) are valid and yield the same results for energies and all other quantities that are invariant under the above phase transformation when examined with an exact method such as QMC. This is not necessarily so when approximations are made as we shall see in the next section.

III. MEAN FIELD PHASE DIAGRAMS

In this section we revisit the mean field phase diagrams of the model governed by Eq. (2) and (3). This is implemented by first writing the identity,

$$a_{\sigma i}^\dagger a_{\sigma j} = \left(a_{\sigma i}^\dagger - \langle a_\sigma^\dagger \rangle \right) \left(a_{\sigma j} - \langle a_\sigma \rangle \right) + \langle a_\sigma^\dagger \rangle a_{\sigma j} + a_{\sigma i}^\dagger \langle a_\sigma \rangle - \langle a_\sigma^\dagger \rangle \langle a_\sigma \rangle. \quad (4)$$

The superfluid order parameter is $\langle a_\sigma^\dagger \rangle = \langle a_\sigma \rangle \equiv \psi_\sigma$ and is taken to be real and uniform, *i.e.* independent of the position. The first term in Eq. (4) is a small fluctuation and is ignored; substituting the remaining terms in Eq. 2 reduces H_1 to the sum of single site Hamiltonians,

$$H_{MF1} = -2td \sum_\sigma (\psi_\sigma (a_\sigma^\dagger + a_\sigma) - \psi_\sigma^2) + \frac{U_0}{2} \sum_\sigma \hat{n}_\sigma (\hat{n}_\sigma - 1) - \frac{|U_2|}{2} \left(a_0^\dagger a_0^\dagger a_\Lambda a_\Lambda + a_\Lambda^\dagger a_\Lambda^\dagger a_0 a_0 \right) + (U_0 + U_2) \hat{n}_0 \hat{n}_\Lambda - \mu \sum_\sigma \hat{n}_\sigma; \quad (5)$$

and from Eq. (3), H_2 becomes

$$\begin{aligned}
H_{MF2} = & -2td \sum_{\sigma} (\psi_{\sigma} (a_{\sigma}^{\dagger} + a_{\sigma}) - \psi_{\sigma}^2) \\
& + \frac{U_0}{2} \sum_{\sigma} \hat{n}_{\sigma} (\hat{n}_{\sigma} - 1) \\
& + \frac{U_2}{2} (a_0^{\dagger} a_0^{\dagger} a_{\Lambda} a_{\Lambda} + a_{\Lambda}^{\dagger} a_{\Lambda}^{\dagger} a_0 a_0) \\
& + (U_0 + U_2) \hat{n}_0 \hat{n}_{\Lambda} - \mu \sum_{\sigma} \hat{n}_{\sigma}. \quad (6)
\end{aligned}$$

The mean field solution is obtained by taking matrix elements of these Hamiltonians in a truncated basis of single site occupation number states $|n_0 n_{\Lambda}\rangle$, diagonalizing the resulting matrix and then minimizing the lowest eigenvalue with respect to the order parameters ψ_{σ} . The basis is truncated for large particles number (typically $n_0 = n_{\Lambda} = 12$) to obtain results independent of the truncation. This gives the order parameters of the ground state and its eigenvector. The superfluid density is given by

$$\rho_s = \psi_0^2 + \psi_{\Lambda}^2. \quad (7)$$

A. Ferromagnetic: $U_2 < 0$

The two mean field Hamiltonians, H_{MF1} and H_{MF2} are identical for the ferromagnetic case, $U_2 < 0$, and their ground state was studied in Ref. [13]. At commensurate filling and strong interaction (small t/U_0) the energy has one minimum at $\psi_0 = \psi_{\Lambda} = 0$ corresponding to the MI. Figure 1(a) shows this for the Mott phase with two particles/site, $\rho = 2$. For any non commensurate filling and for commensurate filling at weak coupling, there are four symmetric and degenerate minima with $|\psi_0| = |\psi_{\Lambda}| \neq 0$ corresponding to the superfluid phase, Fig. 1(d). For later reference, we emphasize that the superfluid phase is symmetric in the two particle species, $|\psi_0| = |\psi_{\Lambda}|$. Figures 1(b,c) show how the minimum at $\psi_0 = \psi_{\Lambda} = 0$ transforms continuously into four degenerate minima visible in Fig. 1(d) as the interaction gets weaker. The same behaviour is seen for the MI at all other commensurate fillings.

The MF phase diagram is obtained by repeating the above calculation for many values of the chemical potential, μ , and the interaction U_0 (always keeping U_2/U_0 constant). In the no-hopping limit, $t/U_0 \rightarrow 0$, it is easy to see that when μ satisfies the condition,

$$(n-1)(U_0 - |U_2|) < \mu < n(U_0 - |U_2|), \quad (8)$$

the system is in a MI phase with n bosons per site. As t/U_0 increases, always keeping $|U_2|/U_0$ constant, the MI region shrinks and eventually disappears giving the familiar Mott lobes. Outside the MI the system is superfluid. Note that U_2 has the effect of shrinking the bases of all the Mott lobes, Fig. 3: When $|U_2| = U_0$ the lobes

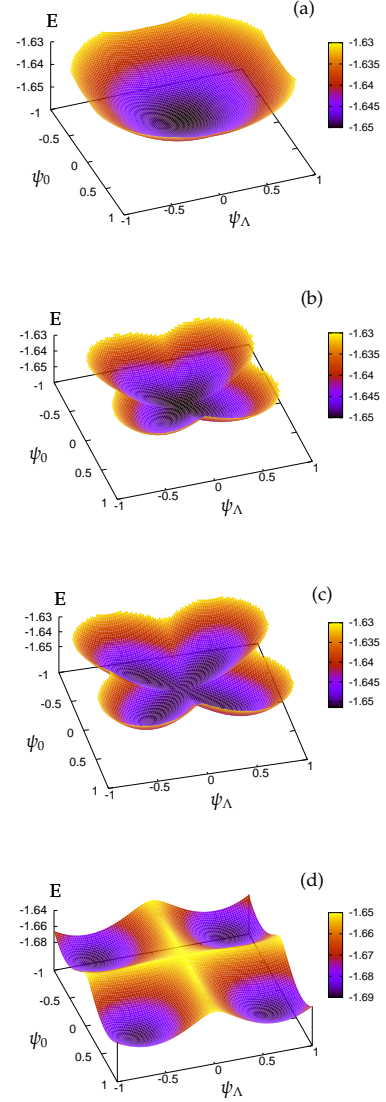


FIG. 1: (Color online) The ground state energy, E , given by Eq. (5) or (6) in the ferromagnetic case, $U_2 = -0.1U_0$ at $\rho = 2$ ($\mu/U_0 = 1.3$). (a) $U_0 = 100t$ the system is in the MI phase. (b) $U_0 = 25t$, the system is in the MI phase close to the transition into the SF phase. (c) $U_0 = 20t$, the system has just made the transition into the SF phase. The minimum has changed continuously from $\psi_0 = \psi_{\Lambda} = 0$ to four degenerate minima at nonzero values of the order parameters. (d) $U_0 = 12.5t$, the system is in the superfluid phase. Note the degenerate symmetric minima in the SF case, $|\psi_0| = |\psi_{\Lambda}| \neq 0$. This figure agrees with Fig. 2 in Ref. [13].

disappear completely. In Fig. 2 we show mean field results for the densities, ρ_0 and ρ_{Λ} of the two species, the total density, $\rho = \rho_0 + \rho_{\Lambda}$ and the corresponding superfluid densities as functions of μ for fixed $t/U_0 = 0.02$ and $U_2/U_0 = -0.1$. We see that all compressible regions, $\kappa = \partial\rho/\partial\mu \neq 0$, are superfluid while the incompressible plateaux, $\kappa = 0$, are not superfluid, they are the MI. The

absence of discontinuous jumps in any of the densities as the system enters the MI indicates the transitions are continuous as also discussed in Ref. [13]. We also remark that since in the ferromagnetic case we have $|\psi_0| = |\psi_\Lambda|$, then $\rho_{s0} = \rho_{s\Lambda}$ and $\rho_0 = \rho_\Lambda$ everywhere except in the first Mott plateau where one of the species has zero density, in this case $\rho_\Lambda = 0$. The reason the first Mott region behaves this way is that in order for the two species to interconvert, the particles have to meet and interact. In the MI phase, the particles do not hop between the sites with the consequence that in the first MI there is only one particle per site and no way to interconvert the species. The phase diagram is shown in Fig. 3.

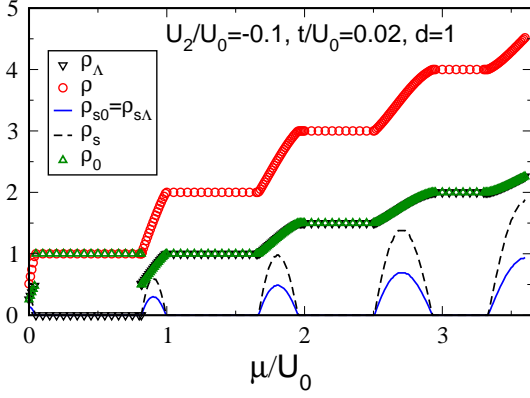


FIG. 2: (Color online) The densities of the two species, ρ_0 and ρ_Λ , the total density, $\rho = \rho_0 + \rho_\Lambda$, and the corresponding superfluid densities as functions of μ/U_0 . In the ferromagnetic case, $\rho_{s0} = \rho_{s\Lambda}$ and $\rho_0 = \rho_\Lambda$ except in the first Mott lobe. The reason is that the particles do not interact and so there is no possibility to convert one species to another.

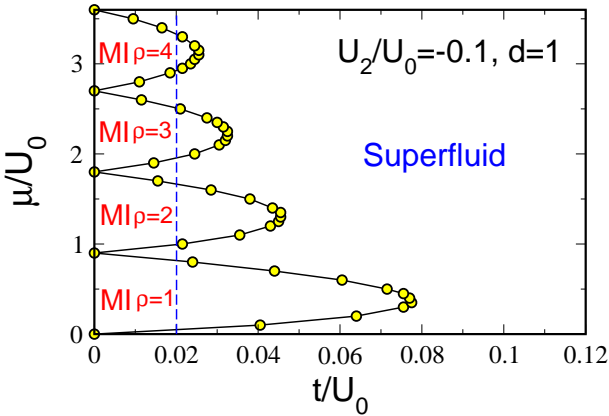


FIG. 3: (Color online) The phase diagram given by the mean field Hamiltonians, Eq. (5) or (6), in the ferromagnetic case $U_2 = -0.1U_0$. Note the shrinking of the bases of all lobes by $|U_2|/U_0$. The dashed vertical line shows where the cut in Fig. 2 was taken.

B. Anti-ferromagnetic: $U_2 > 0$

In the anti-ferromagnetic case, $U_2 > 0$, the Hamiltonians Eq. (5) and Eq. (6) are no longer identical. Reference [13] performed the mean field calculation using Eq. (5) and found that in the MI, the energy has one minimum at $\psi_0 = \psi_\Lambda = 0$. As the system is taken closer to the tip of the Mott lobe, the energy develops local minima (Fig. 6, Ref. [13]); these local minima become global minima in the SF phase indicating that the MI-SF transition can be of first order. Furthermore, it was found that there is a continuum of degenerate minima at nonzero ψ_0 and ψ_Λ (Fig. 6, Ref. [13]).

Doing the mean field calculation with Eq. (6) leads to results which are similar in some ways to the above but different in very important aspects. First, for a given choice of t , U_0 , U_2 and μ , we found that the two mean field Hamiltonians give the same ground state energy both in the SF and MI phases. Therefore, one cannot choose between them on this basis. In the MI phase, whether the filling is odd or even, Eq. (6) gives a ground state energy with one minimum at $\psi_0 = \psi_\Lambda = 0$; the same as Eq. (5). As the system is brought closer to the lobe tip, the behavior depends on whether the filling in the Mott phase is odd or even. Odd filling is similar to the ferromagnetic case: The global minimum at $\psi_0 = \psi_\Lambda = 0$ transforms continuously into four degenerate minima with non-vanishing order parameter. However, in this anti-ferromagnetic case, the minima lie on the ψ_0 and ψ_Λ axes: Either $\psi_0 = 0$ while $\psi_\Lambda \neq 0$, or $\psi_0 \neq 0$ while $\psi_\Lambda = 0$. This means that in the SF phase, the SF density is composed entirely of one species: Either $(\rho_s = \rho_{s0}, \rho_{s\Lambda} = 0)$ or $(\rho_{s0} = 0, \rho_s = \rho_{s\Lambda})$. Our result differs from that in Ref. [13] where a continuum of degenerate minima was found in the SF phase.

If the filling of the MI is even, then as the system approaches the tip of the lobe, decreasing the interaction U_0 , local minima develop at non zero ψ_0 or ψ_Λ : With Eq. (6) the local minima do not form an axisymmetric continuum as they do with Eq. (5), Ref. [13]. As for the odd lobes just discussed, the minima lie either on the ψ_0 axis or on the ψ_Λ axis. This is illustrated in Fig. 4 which shows, for $\rho = 2$, the behaviour of the energy minima as the interaction is reduced taking the system from the MI to the SF phase. Figures 4(b,c) illustrate the behaviour as the system is leaving the MI. First, local minima develop with non-vanishing order parameter, indicating metastable SF, Fig. 4(b). These local minima then become global, for lower U_0 , while the previously global minimum at the origin becomes local indicating that the MI is now metastable, Fig. 4(c). Such behaviour signals a first order SF-MI transition for the even Mott phases. The nature of the transition is in agreement with Ref. [13] but not the nature of the SF phase. According to our mean field result, when the system is in the SF phase, superfluidity is carried entirely by one species or the other but not by both. This result is in marked contrast with that of the MFT based on Eq. (5) and is similar

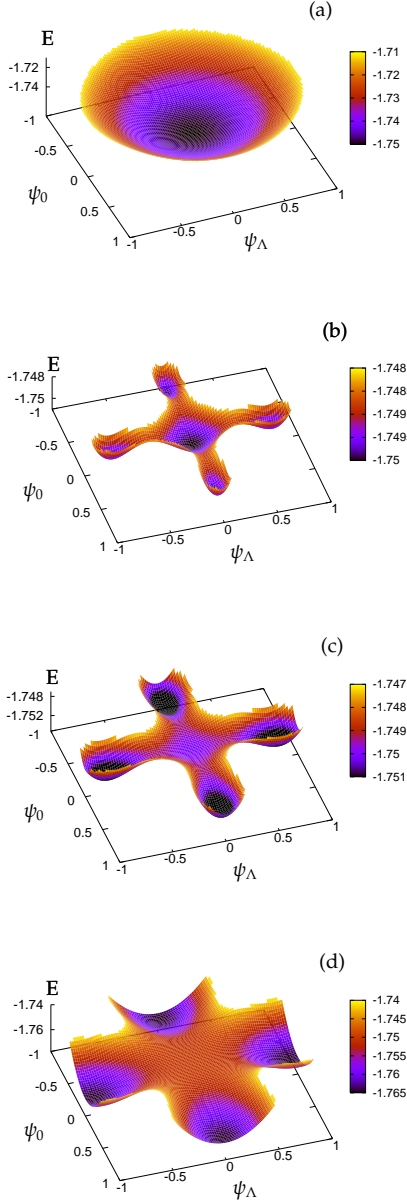


FIG. 4: (Color online) The ground state energy given by Eq. (6) in the anti-ferromagnetic case, $U_2 = 0.1U_0$. (a) $U_0 = 33.3t$, the global minimum is at $\psi_0 = \psi_\Lambda = 0$ and the system is in the MI phase. (b) $U_0 = 12.5t$, the local minima are at non-zero ψ_0 or ψ_Λ indicating stable MI and metastable SF phases. (c) $U_0 = 12.2t$, the global minima are at non-zero ψ_0 or ψ_Λ indicating stable SF and metastable MI phases. (d) $U_0 = 11.1t$, four degenerate global minima indicating the system is in the SF phase.

to the MFT prediction for the SF phase of the full spin-1 model [8] in the antiferromagnetic case.

In Fig. 5 we show the densities of the two species, ρ_0 and ρ_Λ , the total density, $\rho = \rho_0 + \rho_\Lambda$, and the corresponding superfluid densities as functions of μ/U_0 in the anti-ferromagnetic case. Several features are noteworthy.

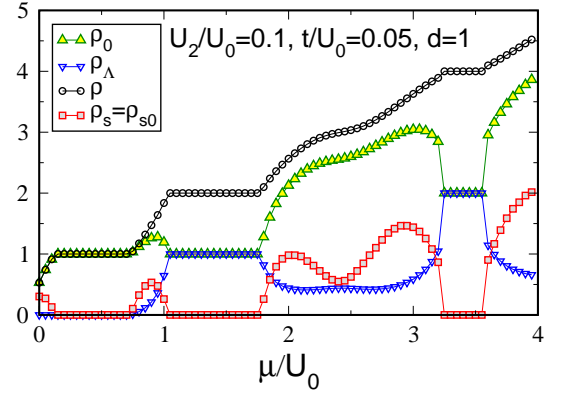


FIG. 5: (Color online) The densities of the two species, ρ_0 and ρ_Λ , the total density, $\rho = \rho_0 + \rho_\Lambda$, and the corresponding superfluid densities as functions of μ/U_0 in the anti-ferromagnetic case. This cut is taken just outside the third lobe (see Fig. 6) so the compressibility, $\kappa = \partial\rho/\partial\mu$, does not quite vanish. Note the discontinuous transition into the fourth Mott lobe.

The first, second and fourth incompressible MI plateaux are clearly visible but the third plateau does not quite form. This is because the cut shown in Fig. 5 passes just outside the third Mott lobe, see the phase diagram Fig. 6. As in the ferromagnetic case, the first Mott lobe is made of only one species, ρ_0 in this case. In the even Mott lobes we have $\rho_0 = \rho_\Lambda$ but nowhere else. In addition, superfluidity is carried entirely by one species; in this case $\rho_s = \rho_{s0}$ and $\rho_{s\Lambda} = 0$ even though $\rho_\Lambda \neq 0$. We also note that the transition into the fourth plateau is discontinuous: We see clearly the discontinuous jumps of ρ_0 , ρ_Λ and ρ_s as this plateau is approached. This is in agreement with the discussion of Fig. 4 and indicates that the system in Fig. 5 enters the fourth Mott lobe near its tip. This is confirmed in the full phase diagram Fig. 6.

The phase diagram is obtained by calculating slices as in Fig. 5 for different values of μ and t/U_0 at fixed U_2/U_0 . Figure 6 shows the mean field phase diagram for the case $U_2 = 0.1U_0$ while the inset shows it for $U_2 = U_0$. The boundaries of the phases do not depend much on whether one uses Eq. (5) or (6) for the mean field calculation. However the nature of the SF phase depends crucially on which Hamiltonian is used as discussed above. For the $U_2/U_0 = 0.1$ case, and more generally for small U_2/U_0 , the transition near the tip of even Mott lobes is first order, as discussed in connection with Figs. 5 and 6: The regions between the squares and the circles around the tips of the even Mott lobes in Fig. 6 denote the regions where the SF (MI) is metastable while MI (SF) is stable. The smaller the ratio U_2/U_0 , the wider the first order transition region. On the other hand, when the ratio U_2/U_0 is large enough, there are no discontinuous transitions; only continuous transitions remain. The extreme case of $U_2 = U_0$, where all odd lobes disappear, is shown in the inset to Fig. 6.

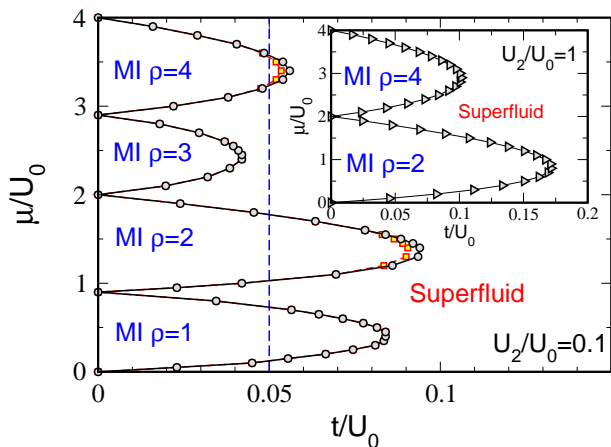


FIG. 6: (Color online) The mean field phase diagram given by Eq. 6 for $U_2/U_0 = 0.1$. The bases of the odd MI lobes are reduced by U_2/U_0 ; the phase transitions near the tips of the even lobes are first order. The regions between the squares and the circles around the tips of the even lobes denote the regions where the SF (MI) is metastable while MI (SF) is stable. Inset: The phase diagram for $U_2/U_0 = 1$: all the odd MI lobes have vanished.

IV. QUANTUM MONTE CARLO PHASE DIAGRAM

In this section we present the results of exact Quantum Monte Carlo simulations for the system governed by the Hamiltonian Eq. (2) or (3). As mentioned before, these two forms of the Hamiltonian are identical for $U_2 < 0$ and are equivalent for $U_2 > 0$ in that they are related by a simple phase rotation and do, in fact, give the same results in QMC simulations for all the quantities we looked at.

We use for our simulations the Stochastic Green Function (SGF) algorithm [15] with directed update [16]. This algorithm can be implemented both in the canonical and the grand canonical ensembles [17]. In this work we used mostly the canonical formulation where we relate the density to the chemical potential using

$$\mu(N) = E(N+1) - E(N). \quad (9)$$

N is the total number of particles in a system with L lattice sites and $E = \langle H \rangle$ is the total internal energy which is equal to the free energy in the ground state. Another very important quantity to characterize the phases is the superfluid density which is given by [18]

$$\rho_s = \frac{\langle W^2 \rangle}{2dt\beta L^{d-2}}, \quad (10)$$

in the single species case where W is the winding number of the bosons. In the present case, there are two species of particles which can be converted into each other. Consequently, the relevant winding number is the total for the

two species and the superfluid density is then given by,

$$\rho_s = \frac{\langle (W_0 + W_\lambda)^2 \rangle}{2dt\beta L^{d-2}}. \quad (11)$$

A. Ferromagnetic case: $U_2 < 0$

We start with ferromagnetic case, $U_2 < 0$. As we did with mean field, we calculate the phase diagram in the $(\mu/U_0, t/U_0)$ plane at fixed ratio U_2/U_0 . We take $|U_2|/U_0 = 0.1$ because we want to use the same value for the ferro- and the anti-ferromagnetic cases and, in the latter case, MFT predicts first order transitions for the even Mott lobes for this value. With $U_2/U_0 = -0.1$, we study the SF-MI transition as the chemical potential (or density) is varied by calculating ρ versus μ slices for different fixed t/U_0 . Using the canonical algorithm, this is done by incrementing the number of bosons by one particle at a time, doing the simulation, and then calculating the chemical potential, μ , using Eq. (9). Figure 7 shows such a slice at $t/U_0 = 0.075$ and clearly exhibits the first two incompressible Mott plateaux. Furthermore, we see that when the system is compressible, it is also superfluid, $\rho_s \neq 0$. In the Mott plateaux, the superfluid density vanishes, $\rho_s = 0$.

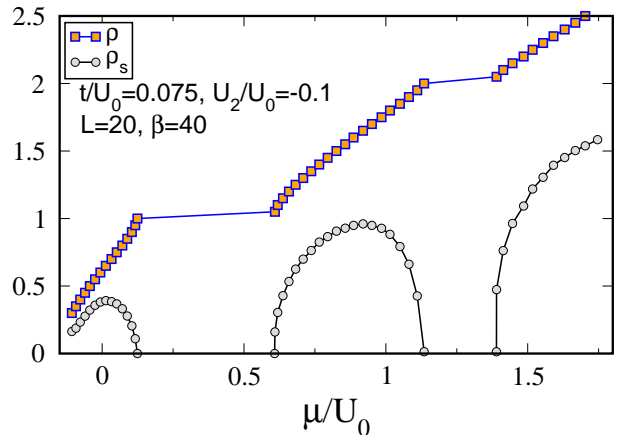


FIG. 7: (Color online) The total particle density, ρ and the superfluid density, ρ_s as functions of the chemical potential, μ . The first two Mott plateaux are clearly visible.

Next, we study the SF-MI transition at fixed commensurate filling, integer ρ , as the coupling, t/U_0 is changed. This exhibits the behaviour of the transition at the tips of the Mott lobes. In Fig. 8 we show the superfluid density, ρ_s versus t/U_0 for $\rho = 1, 2$. We see that in both cases, $\rho = 1$ (Fig. 8(a)) and $\rho = 2$ (Fig. 8(b)), ρ_s changes continuously as predicted by MF.

The phase diagram is obtained by calculating ρ versus μ scans for several t/U_0 values is shown in Fig. 9. System sizes $L = 20, 40, 60$ were used showing very little finite size effects for the gap. We remark that, as expected, the Mott lobes shrink by $\delta\mu/U_0 = 0.1$ at their bases and will

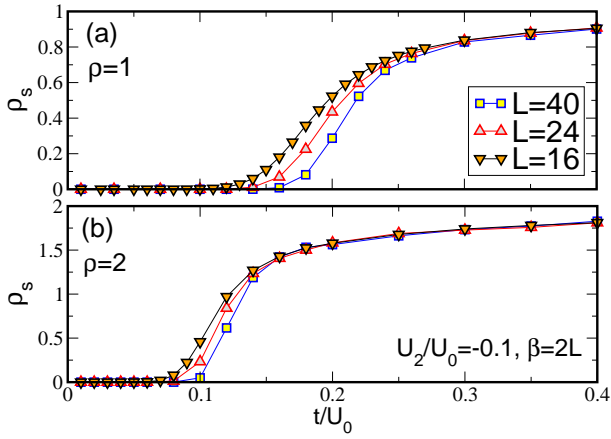


FIG. 8: (Color online) The superfluid density, ρ_s , as a functions of t/U_0 in the first (a) and second (b) Mott lobes. No evidence of a discontinuous jump can be seen as the system size increases, the transitions are continuous.

disappear completely for $|U_2| = U_0 = 1$. While the QMC and MFT phase diagrams are similar qualitatively, the Mott lobes given by the MFT are rounded while those given by exact QMC end in cusps. This is consistent with a critical point at the tip in the universality class of the two-dimensional XY model which is expected from general scaling arguments [20] and first observed in QMC in Ref. [21].

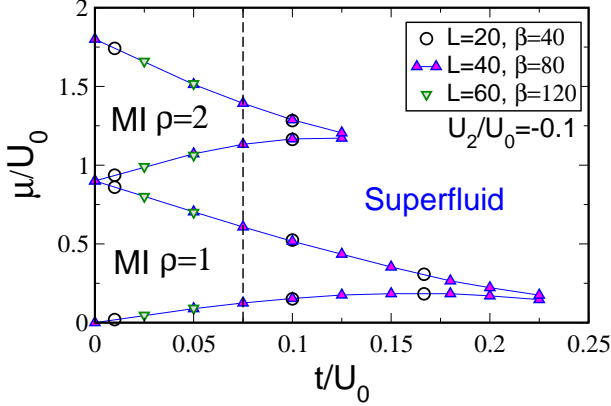


FIG. 9: (Color online) The QMC phase diagram of the ferromagnetic system with $U_2/U_0 = -0.1$. All Mott lobes shrink by $\delta\mu/U_0 = 0.1$ at their bases as in the mean field case, Fig. 3. Note, however, that unlike the rounded lobes in the mean field case, the lobes here end in cusps. This is strong evidence that the gap vanishes exponentially, a behaviour characteristic of the KT universality class of the two-dimensional XY model. This phase diagram is very similar to that of the full spin-1 model in Ref. [9]. The dashed vertical line indicates where the cut in Fig. 7 was taken.

Finally, we show in Fig. 10 the density distribution for total density $\rho = 2$ as t/U_0 is increased taking the system from deep in the second Mott lobe into the superfluid phase as in Fig. 8(b). We find that the distributions for

the 0 and Λ species are identical and that the peak is at $\rho_0 = \rho_\Lambda = 1$ even though the initial state for these simulations was chosen to be $\rho_0 = 2, \rho_\Lambda = 0$: In the ferromagnetic case, the density distributions, $P(\rho_0)$ and $P(\rho_\Lambda)$, are the same both in the MI and SF phases. This means that the superfluid density is carried by both particles. The same behavior was found for $\rho = 1$. This will be compared to the anti-ferromagnetic case below.

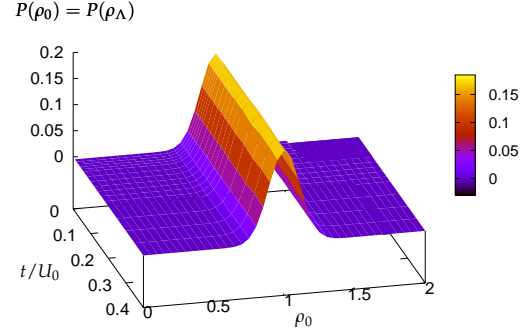


FIG. 10: (Color online) The density distribution of the 0 particles as a function of t/U_0 . The total density is $\rho = 2$ and the values of t/U_0 take the system from deep in the second Mott lobe to the superfluid phase. The distributions of the two species, 0 and Λ , are identical and peak at a value of $\rho/2 = 1$. Compare with Fig. 15.

B. Anti-ferromagnetic case: $U_2 > 0$

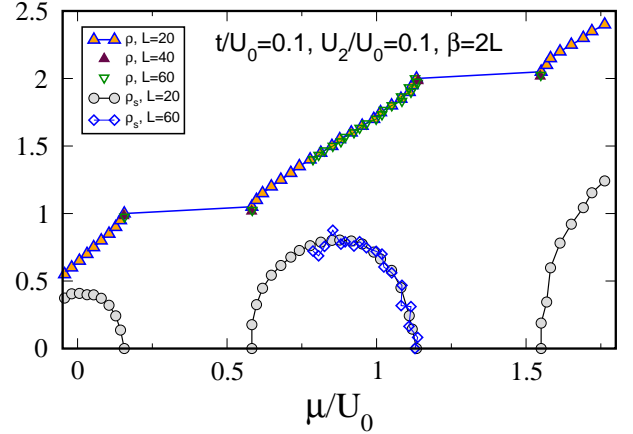


FIG. 11: (Color online) The total density, ρ as a function of the chemical potential, μ , showing the first two incompressible Mott phases. Also shown is the superfluid density ρ_s in the compressible phases.

The phase diagram in the anti-ferromagnetic case, $U_2 > 0$, is determined in the same way as for $U_2 < 0$: We calculate slices of ρ versus μ for various values t/U_0

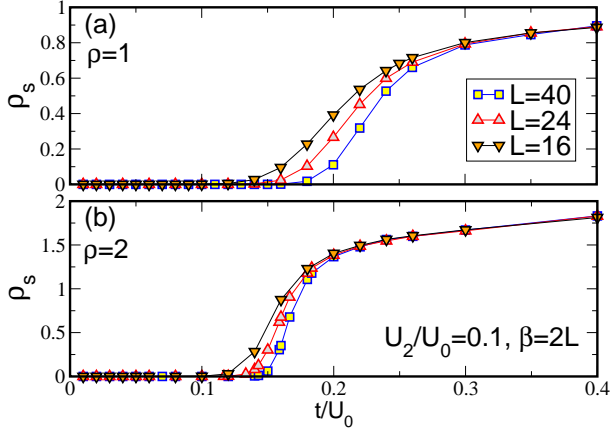


FIG. 12: (Color online) The superfluid density, ρ_s , as a function of t/U_0 in the first (a) and second (b) Mott lobes for the antiferromagnetic case. No evidence of a discontinuous jump can be seen as the system size increases. The SF-MI transitions at the tips of the Mott lobes are continuous.

keeping $U_2/U_0 > 0$ fixed. Such a slice going through the first two Mott plateaux is shown in Fig. 11. As in the ferromagnetic case, we see that the compressible phase is superfluid, $\rho_s \neq 0$. Mean field predicts that the SF-MI transition near the tip of the even Mott lobes is first order. We found no evidence for that; ρ_s vanishes continuously as a function of μ as the MI is approached. In the canonical ensemble, as we have here, first order transitions are signalled by regions of negative compressibility [22], $\kappa = \partial\rho/\partial\mu < 0$. We found that κ is always positive for all values of t/U_0 indicating that the SF-MI transition is not first order.

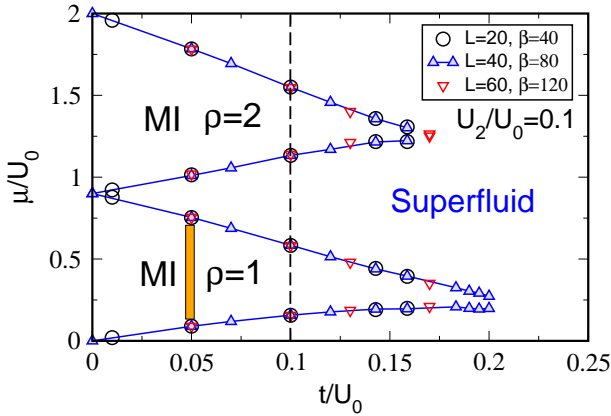


FIG. 13: (Color online) The phase diagram in the antiferromagnetic case with data from three lattice sizes. The finite size effects are small. Note that, as expected, the lower boundary of the base of the second lobe shifts down by $U_2/U_0 = 0.1$ but the upper boundary does not. When $U_2/U_0 = 1$, all odd order lobes disappear and only the even order ones remain. The vertical dashed line indicates where the ρ versus μ cut in Fig. 11 was taken. The vertical (orange) bar at $t/U_0 = 0.05$ in the first lobe indicates where this Mott phase polarizes. See the discussion of Fig. 14.

We confirm the nature of the SF-MI transition by studying the behaviour of the superfluid density as a function of t/U_0 at fixed total density $\rho = 1, 2$. Figure 12 shows ρ_s versus t/U_0 for the first and second Mott plateaux. In both cases ρ_s changes continuously as the system transitions from the MI to the SF phase confirming that all SF-MI transitions in this model are continuous.

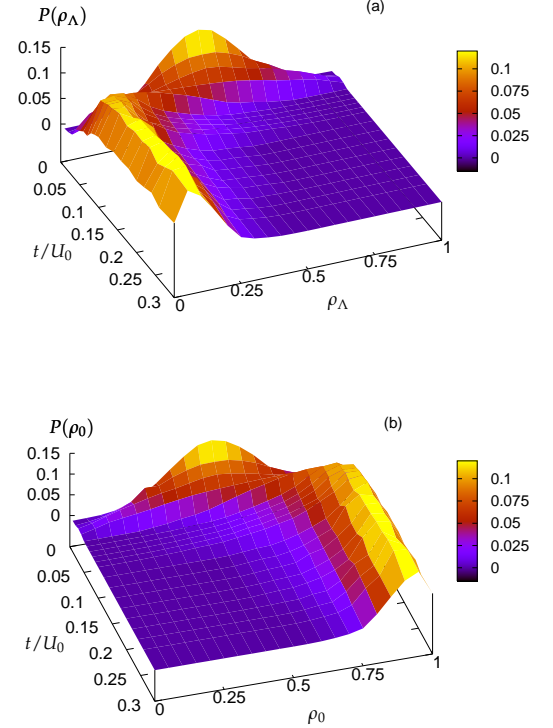


FIG. 14: (Color online) The density distribution of the Λ (a) and 0 (b) particles as functions of t/U_0 . The system size is $L = 40$, $\beta = 80$, and the total density is $\rho = 1$. The values of t/U_0 take the system from deep in the first Mott lobe to the superfluid phase. Inside the Mott lobe, the system is unpolarized, $P(\rho_0) = P(\rho_\Lambda)$, for $t/U_0 < 0.05$ and both distributions peak at $\rho/2 = 0.5$. At $t/U_0 \approx 0.05$, while the system is still in the first Mott lobe, it polarizes: The peak of one distribution approaches the total density, $\rho = 1$, while the other approaches 0. We verified that the same behaviour is observed for different system sizes. This transition in the Mott lobe is not predicted by MF.

The phase diagram is obtained, as before, by calculating ρ versus μ for several values of t/U_0 and mapping out the Mott lobes. The resulting phase diagram for the first two lobes is shown in Fig. 13.

Finally, we show in Fig. 14 that the density distribution for total density $\rho = 1$ as t/U_0 is increased taking the system from deep in the first Mott lobe into the superfluid phase. We see that for $t/U_0 < 0.05$, the system is unpolarized, the two populations have identical distribu-

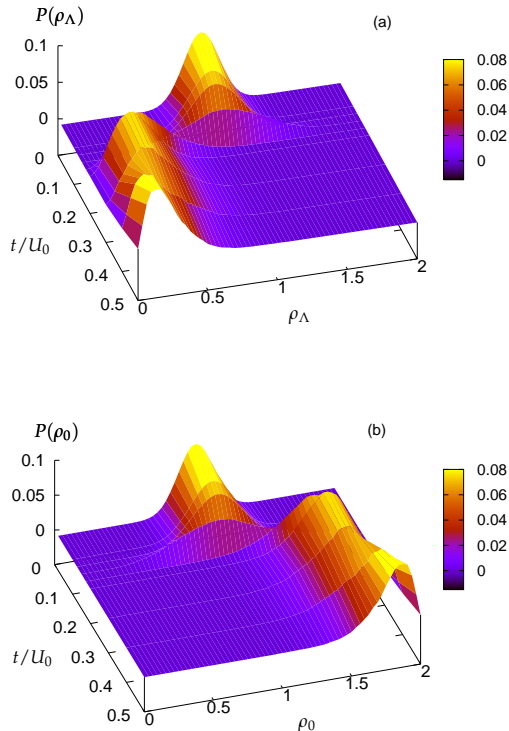


FIG. 15: (Color online) The density distribution of the Λ (a) and 0 (b) particles as functions of t/U_0 . The system size is $L = 64$, $\beta = 128$, and the total density is $\rho = 2$ and the values of t/U_0 take the system from deep in the second Mott lobe to the superfluid phase. Inside the Mott lobe, $P(\rho_0) = P(\rho_\Lambda)$ and both distributions peak at $\rho/2 = 1$. As soon as the system leaves the Mott phase and becomes superfluid, it is polarized: The peak of one distribution approaches the total density, $\rho = 2$, while the other approaches 0. The superfluid phase is polarized as predicted by the MFT: the superfluidity is carried entirely by one species.

tions which peak at $\rho_\Lambda = \rho_0 = 0.5$. At $t/U_0 \approx 0.05$, while the system is still deep in the Mott lobe (see Fig. 13) the system polarizes: The population of one species drops abruptly to near zero while that of the other species increases to close to full filling. This polarization persists

through the SF-MI transition. This transition inside the first Mott lobe is not predicted by mean field.

In Fig. 15 we show the density distributions in the second Mott lobe. Here we find that the system polarizes only when it transitions from the MI to the SF phase at $t/U_0 \approx 0.17$. Consequently, the SF phase in the antiferromagnetic phase is always polarized: The system is mostly populated by a single species and, consequently, superfluidity is carried by that one particle type. This behaviour was predicted, qualitatively, by our mean field calculation and is very different from the behavior in the ferromagnetic case.

V. CONCLUSIONS

In this work, we performed a mean field calculation of the phase diagram of the spin-1/2 bosonic Hubbard model, Eqs. (2 and 3). These models, which are derived from the full spin-1 model, are equivalent when treated exactly but we found that the mean field results depend on which Hamiltonian is used in the antiferromagnetic ($U_2 > 0$) case but are identical in the ferromagnetic case ($U_2 < 0$). Unlike a previous mean field result [13] we found the superfluid phase is polarized when $U_2 > 0$. We then used QMC to calculate the phase diagram for $U_2 < 0$ and $U_2 > 0$. For $U_2 < 0$, we found that the populations are balanced both in the superfluid and in the incompressible phases. For $U_2 > 0$, we found that the SF phase is always polarized with one species dominating the population. Throughout the second Mott lobe (and presumably in all even Mott lobes) the populations are balanced. On the other hand, for $t/U_0 < 0.05$ in the first Mott lobe, we found that the populations are balanced but that the system polarizes inside the Mott lobe at $t/U_0 \approx 0.05$. This new transition inside the Mott lobe was not predicted before.

Acknowledgments

This work was supported by: the CNRS-UC Davis EPOCAL LIA joint research grant; by NSF grant OISE-0952300; an ARO Award W911NF0710576 with funds from the DARPA OLE Program; We thank A. Brothers for helpful insight.

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